## XML for Microanalysis

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**CSTL researcher creates new microanalysis technique schemas for AnIML covering spectroscopies and electron optical scanning techniques (STEM, SEM, Spectrum Imaging).**

The rapid spread of XML technology in many fields of chemical analysis has led to renewed interest in applying XML to the data exchange and data storage problems faced by the microanalysis community. Information about all aspects of a microanalysis experiment (not just spectral results) can be captured by a well-designed Microanalysis Markup Language (MML), which should:

- Enable the free exchange of spectral information among microanalytical instrument users by developing an XML-compliant markup language for spectroscopy data.
- Provide a framework for sharing microanalysis data community-wide to allow more sophisticated theoretical model building and model assessment to take place.
- Create a document format for long-term archiving of microanalysis data that diminishes the effect of "bit-rot" and software decay and helps prevent the loss of data due to lost file formats.

After testing several variation of the markup language and exploring design tradeoffs, as well as implementing multiple working prototypes to store test data, we began to integrate the microanalysis XML effort into the ASTM E13.15 AnIML, which is the analytical data markup language project also CSTL-led but by an independent team as described in the previous article. The two projects can interoperate cleanly and a microanalysis component can be added to the AnIML project through the development of technique schemas (defined by the AnIML framework) based on common microanalysis data acquisition modalities such as scanning transmission electron microscope (STEM), scanning electron microscopy (SEM), and elemental analysis spectroscopies such as electron energy-loss spectroscopy (EELS) and energy-dispersive x-ray spectrometry (XEDS).

This year we implemented multiple working prototypes of Microanalysis Markup Language (MML) based on the original ASCII file format created in 1991 by the Electron Microscopy Society of America (EMSA) task force, currently the Microscopy Society of America (MSA). The larger CSTL team began to integrate concepts from SpectroML and AnIML, and began contributing to AnIML development by attending meetings, studying the schema and framework, and learning the role of ASTM Analytical Data Sub Committee E13.15. We estimate that the creation of new microanalysis technique schemas for AnIML covering spectroscopies and electron optical scanning techniques (STEM, SEM, Spectrum Imaging) will add significantly to their schema list while the XML-based metadata is already useful for storing information about spectrum imaging experiments to complement LISPIX .rpl files and 3D Chemical Imaging competence.

```
#FORMAT      : EMSA/MAS Spectral Data
File
#VERSION     : 1.0
#TITLE       : NIO EELS OK SHELL
#DATE        : 01-OCT-1991
#TIME        : 12:00
#OWNER       : EMSA/MAS TASK FORCE
#NPOINTS     : 20.
#NCOLUMNS    : 1.
#XUNITS      : Energy Loss (eV)
#YUNITS      : Intensity
#DATATYPE    : XY
#XPERCHAN    : 3.1
#OFFSET      : 520.13
#CHOFFSET    : -168
#SIGNALTYPE  : ELS
#XLABEL      :  Energy
#YLABEL      :  Counts
#BEAMKV   -kV: 120.0
#EMISSION -uA: 5.5
```

**Example file excerpts from the headers of the existing EMSA/MAS Spectrum File Format 1.0 (top), and Microscopy Markup Language (MML), a proposed XML-based enhanced format (bottom). Both formats are designed to be human-readable/editable and intuitive instead of efficient and parsimonious. The XML-based format has the added advantages of being extensible, web-aware, more easily validated, and more tolerant of vendor customization. It is also backed by a large, professionally-developed codebase, a suite of tools, and plentiful documentation on XML itself.**

```
<?xml version="1.0"?>
<spectrum xunits="Energy Loss (eV)"
yunits="Intensity" signaltype="ELS">
<title>NIO EELS OK SHELL</title>
<date>1991-10-01</date>
<time>12:00</time>
<owner>EMSA/MAS TASK FORCE</owner>
<xperchan>3.1</xperchan>
<offset>520.13</offset>
<choffset>-168</choffset>
<beamkv>120.0</beamkv>
<emission-uA>5.5</emission-uA>
<probecurrent-nA>12.345</probecurrent-
nA>
```

In the coming year we plan to extend and refine the standard to resolve remaining questions while developing a more detailed model for XML use in spectrum imaging applications. We would also like to explore the use of XML in building a data pipeline for 3D Chemical Imaging at the Nanoscale.